Modelling of Time-Resolved X-ray Diffraction from Laser-Shocked Crystals

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High power lasers with nanosecond pulse-lengths can be used to launch shock waves into solids. A separate arm of the same laser can be focused to extremely high irradiances, forming a plasma which is a copious source of quasi-monochromatic X-rays with pulse durations of order a nanosecond. These X-rays can be diffracted from the crystal during the passage of the shock wave, providing direct information on the degree of elastic strain present within the sample.

Unlike synchrotron radiation, the X-ray emission from the plasma is fully divergent. In order to obtain information on the state of the crystal from reflections from multiple planes, a large angle detector is required. The recording of the transient changes in lattice spacings of planes both parallel and perpendicular to the shock propagation direction is of particular importance. As the shock is uniaxial, the total transverse strain is zero. However, under high pressure shock compression, above the so-called Hugoniot elastic limit, materials start to behave hydrostatically, and presumably this must be recordable in the diffraction signal by an observed compression of the lattice in all directions, despite the unixial strain conditions. Indeed this is the case – X-rays are sensitive to elastic strain, and in the direction transverse to the shock, the elastic strain is equal and opposite to the plastic strain caused by the generation and motion of dislocations. Hence X-ray diffraction can give direct information on the degree of plastic deformation within the shocked sample.

The precise mechanisms by which materials can deform plastically at ultrahigh strain rates ($\sim 10^9$ s^{-1}) have been a matter of debate for many decades. New light has started to be shed on this area with the advent of multi-million atom molecular dynamics simulations, which have revealed some of the dynamics of how homogeneous dislocation generation takes place in shocked metal crystals on picosecond timescales.[1] Post-processing of the molecular dynamics simulations to provided calculated diffraction patterns show that indeed the unit cell can quickly relax towards hydrostatic conditions, but the rate at which this takes place is dependent on the purity of the crystal and its defect content.

The simulations are consistent with experimental data which shows deformation in all directions under shock compression of the unit cell of copper - see Fig. 1 (c) and (d).

The timescale for deformation is consistent with predicted dislocation densities and velocities. In contrast covalently bonded materials, such as silicon, exhibit markedly different behaviour, apparently remaining purely elastic on nanosecond timescales even under shock compression of the lattice as large as 11%, [2] as shown in part (a) and (b) of the figure (in this figure 'Bragg' corresponds to diffraction from planes with reciprocal lattice vectors parallel to the shock propagation direction, whereas 'Laue' are planes with reciprocal lattice vectors perpendicular to the shock). Full details of the experiment can be found in reference 2.

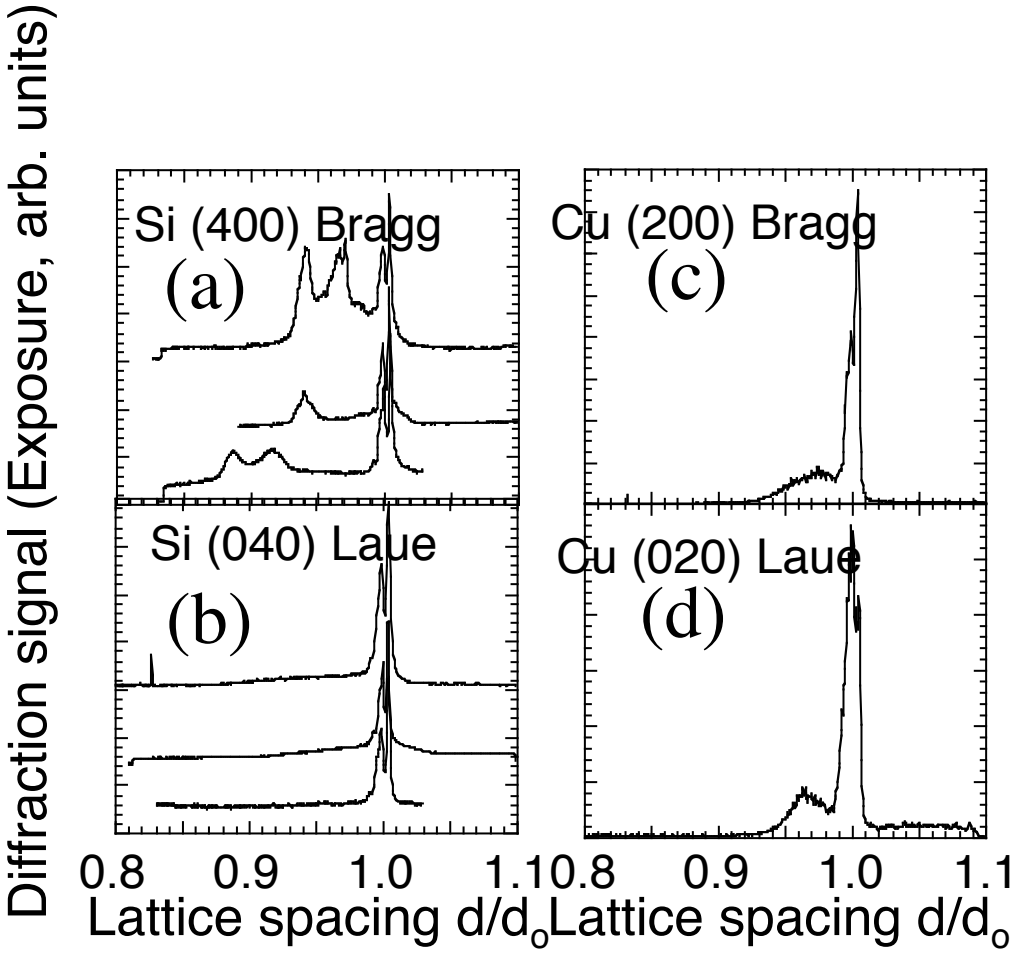

Fig. 1: Diffraction from laser-shocked silicon and copper. The shock propagates along the x-axis. Note that compression is seen in copper for planes both perpendicular and parallel to the shock, indicating plastic flow on sub-nanosecond timescales, whereas silicon apparently exhibits fully elastic behaviour.

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[2] A.Loveridge-Smith, A. Allen, J Belak, T. Boehly, A. Hauer, B. Holian, D. Kalantar, G. Kyrala, R.W. Lee, P. Lomdahl, M.A. Meyers, D. Paisley, S. Pollaine, B. Remington, D.C. Swift, S. Weber, J.S. Wark, Phys. Rev. Lett. **86**, 2349 (2001).